Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Comparative Studies of the Energetic and Properties of gamma-GeSi2N4 and gamma-SiGe2N4 in the Spinel Structure HONGZHI YAO, LIZHI OUYANG, WAI-YIM CHING — To resolve the controversy on the issue about the preferred site of A and B in Si-Ge double nitride that have geometrically ternary structure form of AB_2X_4, where A and B are cations at the tetrahedral and octahedral sites respectively and X is an anion, we have calculated phonon spectrum and thermodynamic properties of Si-Ge spinel nitride solid solutions by first-principles density functional method using both unit and 2*2*2 supercells. Our new results showed that γ-GeSi2N4 is more stable than γ-SiGe2N4 based purely on formation energy calculation. However, the vibrational contribution shows opposite effects. The vibrational contribution to free energy is rather small at room temperature, but at 2000K, it makes a sizable contribution, of the order of 10 eV/atom, to the free energy. Therefore, the experimentally observed stable phase is likely the results of this two competing effects. We have also carried out a detailed ab-initio calculation of all independent elastic constants for Si-Ge spinel nitride systems. The results will be compared to the experimental measurements and some other calculations.

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Date submitted: 30 Nov 2004 Electronic form version 1.4